First order quantum phase transitions of the XX spin-$1/2$ chain in a uniform transverse field

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Abstract

Quantum phase transitional behavior of a finite periodic XX spin-$\frac{1}{2}$ chain with nearest neighbor interaction in a uniform transverse field is studied based on the simple exact solutions. It is found that there are $[N/2]$ level-crossing points in the ground state, where N is the periodic number of the system and $[x]$ stands for the integer part of x, when the interaction strength and magnitude of the magnetic field satisfy certain conditions. The quantum phase transitions are of the first order due to the level-crossing. The ground state in the thermodynamic limit will be divided into three distinguishable quantum phases.

Keywords: XX spin chain, level-crossings, quantum phase transition, ground state entanglement

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It is well known that the finite periodic XX spin-$\frac{1}{2}$ chain with nearest neighbor interaction in a uniform transverse field is simply solvable. The result was first reported by Lieb et al, and then by many others.[2−6] Similar models have been attracted a lot of attention recently due to the fact that they may be potentially helpful in quantum information processing[7−9] and realizable by using quantum dots, optical lattice, or spin interaction systems.[10−12] These spin systems usually undergo quantum phase transitions (QPTs) under certain conditions at zero temperature, which can be characterized by non-analyticity in properties of the ground state.[13] There are intimate links between QPTs and entanglement in the systems.[9,14−16] In this Letter it will be shown that there are a series of level-crossing points when the interaction strength and magnitude of the magnetic field satisfy certain conditions, and the entanglement measure[17,18] defined in terms of von Neumann entropy of one-body reduced density matrix can be used to indicating both the multi-particle entanglement and QPTs in the system.

The Hamiltonian of the model can be written as

$$\mathcal{H}_{\rm XX} = -J\sum_{i=1}^{N}\left(S_i^+S_{i+1}^- + S_{i+1}^+S_i^-\right) + h\sum_{i=1}^{N}S_i^0, \tag{1}$$

where S_i^μ ($\mu=+,-,0$) are spin operators satisfying the SU(2) commutation relations: $[S_i^0, S_j^\pm] = \delta_{ij}S_j^\pm$, $[S_i^+, S_j^-] = 2\delta_{ij}S_j^0$, $J>0$ is the nearest neighbor interaction strength, h is a uniform transverse field, and the periodic condition $S_{i+N}^\mu = S_i^\mu$ is assumed. These spin operators can be realized by the periodic-N hard-core boson operators with $S_i^+ \to b_i^\dagger$, $S_i^- \to b_i$, and $S_i^0 \to b_i^\dagger b_i - \frac{1}{2}$, which satisfy $[b_i, b_j^\dagger] = \delta_{ij}(1-2b_j^\dagger b_j)$, $[b_i^\dagger, b_j^\dagger] = [b_i, b_j] = 0$, and $(b_i)^2 = (b_i^\dagger)^2 = 0$. Thus, up to a constant, (1) can be rewritten as

$$H_{\rm XX} = -\frac{1-t}{2}\sum_{i=1}^{N}\left(b_i^\dagger b_{i+1} + b_{i+1}^+ b_i\right) + \frac{t}{2}\sum_{i=1}^{N} b_i^\dagger b_i, \tag{2}$$

where, in order to investigate QPT behavior of the system, we have set $J=(1-t)/2$ and $h=t/2$ with $0\le t\le 1$. Though the neglected constant term in (2) is dependent on t, it only results in a slight change in the positions of critical points, and the phase transitional behavior of the system keeps unchanged. It is clear that the ground state of the system is in the ferromagnetic (unentangled) phase when $t=1$ and in the long-range order (entangled) phase when $t=0$. Therefore, t serves as the control parameter of the system. By using the results shown in Refs. [1-6], the k-'particle' wavefunctions of (2) can be expressed as

$$|k;(i_1 i_2 \cdots i_k)\rangle = A^\dagger_{i_1} A^\dagger_{i_2} \cdots A^\dagger_{i_k}|0\rangle \tag{3}$$

with $1 \le i_1 \ne i_2 \ne \cdots \ne i_k \le N$, where $|0\rangle$ is the boson vacuum and thus the SU(2) lowest weight state with $S^-_i|0\rangle = 0\ \forall\ i$, and $A^\dagger_\mu = \sum_{j=1}^N c_j^{(\mu)} b^\dagger_j$ with

$$c_j^{(\mu)} = \begin{cases} e^{\imath 2\pi\mu j/N} & \text{for } k = \text{odd}, \\ e^{\imath\pi(2\mu+1)j/N} & \text{for } k = \text{even} \end{cases} \tag{4}$$

corresponding to the μ-th set of eigenvectors of the matrix with $\sum_{i=1}^{N-1}(E_{ii+1} + E_{i+1i}) - (-1)^k(E_{1N} + E_{N1})$, in which E_{ij} are the matrix units or generators of $U(N)$ in the fundamental representation. The corresponding eigen-energy of (3) is

$$E^k(t) = \sum_{\mu=1}^{k} \epsilon_{i_\mu}(t) \quad \text{with} \quad \epsilon_{i_\mu}(t) = \begin{cases} \epsilon(\mathrm{o}\ , i_\mu, t) = -(1-t)\cos\frac{2\pi i_\mu}{N} + t/2 & \text{for } k = \text{odd}, \\ \epsilon(\mathrm{e},\ i_\mu, t) = -(1-t)\cos\frac{\pi(2i_\mu+1)}{N} + t/2 & \text{for } k = \text{even} \end{cases} \tag{5}$$

with $N \ge 2$. Though the above results are analytic, it is still not easy to write out those corresponding to a specific state explicitly, especially to the ground state, from (3),(4), and (5) directly. However, we have verified that the ground state energy for periodic-N chain is related to the following set of eigen-energies:

$$E^k_{\min}(t) = \begin{cases} \sum_{i=1}^{[k/2]} \epsilon(\mathrm{o},\ i, t) + \sum_{i=0}^{[k/2]} \epsilon(\mathrm{o},\ N-i, t) & \text{for odd } k, \\ \sum_{i=1}^{[k/2-1]} \epsilon(\mathrm{e},\ i, t) + \sum_{i=0}^{[k/2]} \epsilon(\mathrm{e},\ N-i, t) & \text{for even } k \end{cases} \tag{6}$$

with $k = 0, 1, \cdots, [N/2]$, where $[x]$ stands for the integer part of x. It should be stated that the ground state energy at $t = 1$ corresponds to $E^0_{\min}(t) = 0$ from (6), while that at $t = 0$ corresponds to $E^{[N/2]}_{\min}(t)$. Hence, it is clear that there are $[N/2]+1$ different set of mutually orthogonal states with the corresponding ground state energy $E^{[N/2]}_{\min}(t)$, $E^{[N/2]-1}_{\min}(t)$, $\cdots$, $E^1_{\min}(t)$, $E^0_{\min}(t)$, respectively, when the control parameter t changes from 0 to 1. Such quantum phase transitions are of the first order because the first derivative of the ground state energy to the control parameter t is discontinuous at the critical point, $\lim_{t\to t_\mathrm{c}-0} \frac{\partial E_\mathrm{g}(t)}{\partial t} \ne \lim_{t\to t_\mathrm{c}+0} \frac{\partial E_\mathrm{g}(t)}{\partial t}$, according to the extended Erhenfest classification of phase transitions.[19]

Table 1. First 9 level-crossing points for different N cases in addition to $t_\mathrm{c}^{(0)}$.

N	$t_\mathrm{c}^{(1)}$	$t_\mathrm{c}^{(2)}$	$t_\mathrm{c}^{(3)}$	$t_\mathrm{c}^{(4)}$	$t_\mathrm{c}^{(5)}$	$t_\mathrm{c}^{(6)}$	$t_\mathrm{c}^{(7)}$	$t_\mathrm{c}^{(8)}$	$t_\mathrm{c}^{(9)}$
4	0.453082								
6	0.594173	0.348915							
8	0.629014	0.531157	0.284603						
10	0.643395	0.588789	0.478976	0.240565					
12	0.650802	0.615444	0.551173	0.435657	0.208426				
14	0.655138	0.630200	0.587316	0.517094	0.399305	0.18390			
16	0.657902	0.639299	0.608381	0.560425	0.486483	0.36843	0.16456		
18	0.659775	0.645332	0.621866	0.586711	0.535216	0.45901	0.34193	0.1489	
20	0.661103	0.649550	0.631072	0.604041	0.565767	0.51177	0.43430	0.31895	0.13599
100	0.666447	0.666008	0.665347	0.664462	0.663352	0.66201	0.66043	0.65862	0.65657
1000	0.666664	0.66666	0.666654	0.666645	0.666634	0.66662	0.66660	0.66658	0.66656

The first order phase transition in the system occurs due to the ground state energy level-crossing of $E^i_{\min}(t)$ with $E^{i+1}_{\min}(t)$ for $i = 0, 1, \cdots, [N/2]-1$ with the corresponding critical point $t_\mathrm{c}^{(i)}$, which is the root of the simple linear equation $E^i_{\min}(t_\mathrm{c}^{(i)}) = E^{i+1}_{\min}(t_\mathrm{c}^{(i)})$ for $i = 0, 1, 2, \cdots, [N/2]-1$. Hence, there are

$[N/2]$ critical points within the control parameter range $0 \leq t \leq 1$. Fig. 1 clearly shows the ground state level crossings in the entire control parameter range for $N = 6,\ 8,\ ,20$ and 100 cases. It is obvious that there are $[N/2]$ level-crossing points dividing the ground state into $[N/2]+1$ different parts, of which each is within a specific t range when N is a finite number. With N increasing, however, these specific ranges become smaller and smaller, and finally tends to infinitesimal, thus the ground state level becomes a continuous phase before crossing to $E^0_{\rm min}$ level. Therefore, there will be only one obvious critical point when $N \rightarrow \infty$. Since $E^1_{\rm min}(t) = 3t/2 - 1$ for any N, the obvious critical point is at $t_{\rm c}^{(0)} = 2/3$ in the thermodynamic limit. Nevertheless, other level-crossing point $t_{\rm c}^{(i)}$ values in the finite N cases are N-dependent, of which some examples are listed in Table 1.

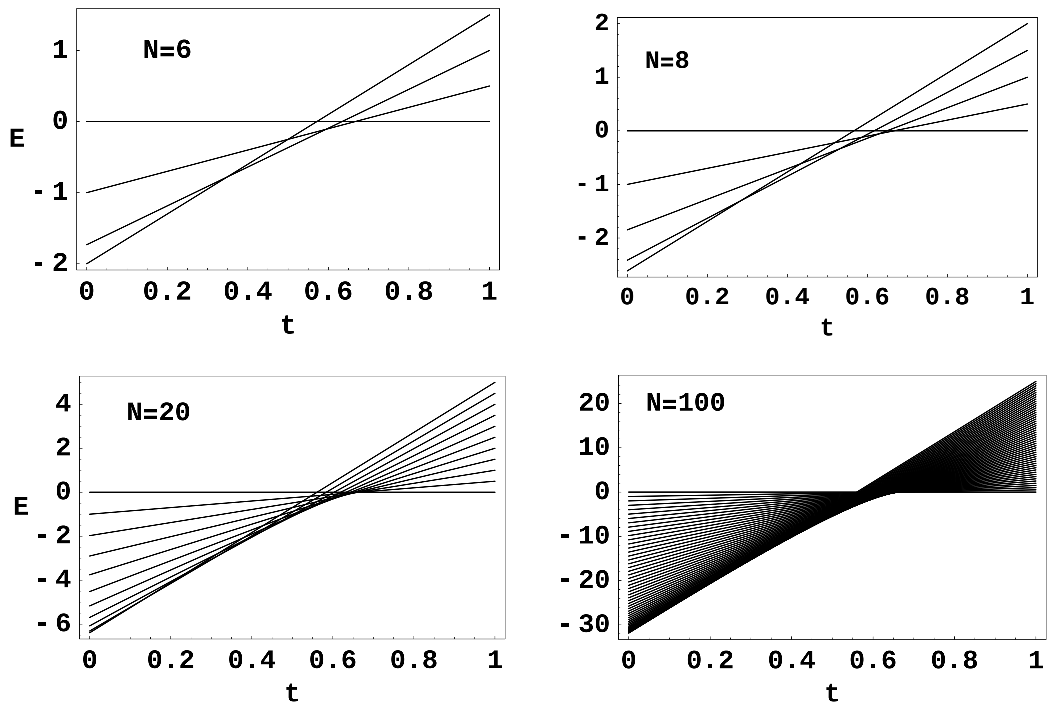

Figure 1: Level crossings related to the ground state for different N cases.

Entanglement in the model is often studied by using block–block entanglement defined in terms of von Neumann entropy[15] or Wootters concurrence[20], e. g., that shown in [21]. In the following, we use the simple measure proposed in [17] with

$$\eta(\Psi) = -\frac{1}{N}\sum_{i=1}^{N} {\rm Tr}\left\{(\rho_\Psi)_i \log(\rho_\Psi)_i\right\} \tag{7}$$

if all N terms in the sum are non-zero, otherwise $\eta(\Psi) = 0$, where Ψ stands for the ground state wavefunction and $(\rho_\Psi)_i$ is the reduced density matrix with the i-th site only. It has been shown[18,22,23] that (7) is also suitable to measure genuine N-body entanglement. We observed that $(\rho_\Psi)_i$ is independent of i for the ground state in the model. Hence, the entanglement measure η can be simply defined by the reduced von Neumann entropy for any site in this case. Table 2 shows ground state entanglement in different t ranges for $N = 2, \cdots, 6$, respectively, in which the entanglement type of the ground state in each range is indicated. For example, the state is a linear combination of several GHZ-like states for $N = 4$ with $0 \leq t < 0.453082$, while it is a linear combination of serval W-like states for $N = 5$

with $0 \leq t < 0.552786$. It is clear that the ground state entanglement measure gradually increases while the control parameter t decreases, which is also characterized by the quantum number $S^0 = \sum_i S_i^0$. In the separable ferromagnetic phase, S^0 reaches its lowest value with $S^0 = -N/2$, while it becomes close to 0 when $t < t_c^{[N/2]}$, in which the spin-up and -down fermions are most strongly correlated in comparison to that in other cases. In the most entangled long-range order phase, even-N systems are most entangled with $\eta = 1$ which is always greater than those of the nearest odd-N systems. Furthermore, the ground state is not degenerate if the control parameter t does not at those $[N/2]$ level-crossing points, while it becomes two-fold degenerate when $t = t_c^{(i)}$ for any i as far as these states are concerned, which is mainly due to the S_2 permutation symmetry defined by the permutation of two sets of sites with $\{1, 2, \cdots, [N/2]\} \rightleftharpoons \{N-1, N-2, \cdots, N-[N/2]\}$. Nevertheless, these pairs of degenerate states are still distinguishable from each other by the quantum number S^0 with their difference $\Delta(S^0) = \pm 1$ and by values of the entanglement measure of these two degenerate states. As a consequence, the ground state in the thermodynamic limit is not degenerate when $t = 0$; it becomes two-fold degenerate everywhere when the control parameter t is within the half-open interval $t \in (0, 2/3]$ because the level-crossing points are dense everywhere in this control parameter range in the $N \to \infty$ limit; and finally it becomes non-degenerate again when $2/3 < t \leq 1$. Therefore, the ground state should be classified into three phases rather than two in the thermodynamic limit. These three phases are one entangled GHZ-type phase at $t = 0$ with $\eta = 1$, one degenerate entangled W-type phase with $t \in (0, 2/3]$ and $0 < \eta < 1$, and one non-degenerate fully separable phase with $t \in (2/3, 1]$ and $\eta = 0$. It has been proved at least for small N cases that GHZ- and W-type states are inequivalent under the SLOCC transformations.[22–24] We call the quantum phase at $t = 0$ hidden because the first derivative of the ground state energy seems continuous at $t \in [0, \epsilon \to 0)$.

Table 2. Ground state entanglement with each quantum phase for $N = 2, \cdots, 6$

N	Entanglement type in each phase			
2	Fully separable ($\eta = 0$) $2/3 < t \leq 1$	Bell ($\eta = 1$) $0 \leq t < 2/3$		
3	The same as above	W ($\eta = 0.918296$) $0 \leq t < 2/3$		
4	The same as above	W ($\eta = 0.811278$) $0.453082 < t < 2/3$	GHZ Combination ($\eta = 1$) $0 \leq t < 0.453082$	
5	The same as above	W ($\eta = 0.721928$) $0.552786 < t < 2/3$	W combination ($\eta = 0.970951$) $0 \leq t < 0.552786$	
6	The same as above	W ($\eta = 0.650022$) $0.594173 < t < 2/3$	W Combination ($\eta = 0.918296$) $0.594173 < t < 0.348915$	GHZ Combination ($\eta = 1$) $0 \leq t < 0.348915$

In summary, the ground state of the finite periodic-N XX spin-$\frac{1}{2}$ chain with nearest neighbor interaction in a uniform transverse field is revisited by using the simple exact solutions. The energy eigenvalues and the corresponding eigenstates related to the ground state of the system are obtained analytically. The results show how the ground state of the model evolves from the ferromagnetic phase to the anti-ferromagnetic long-range order phase with decreasing of the control parameter t introduced. In addition, we have shown that there are $[N/2]$ level-crossings in the system, in which the middle part of long-range order phases will become a continuous one in the large-N limit leading to the three-phase result in the thermodynamic limit. Such level-crossing was also observed from a numerical study for specific N cases of

XY spin chain,[25] and should be common in other spin interaction systems in a uniform transverse field. Obviously, our analytic and finite N analysis provide with the microscopic structure of the ground state of the model. Similar analysis for other spin chain models may also be helpful, which will be discussed elsewhere.

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